169801

Arcess DBII

SEARCH REQUEST FORM

Scientific and Technical Information Center

REMSAIO, SC/R If more than one search is submitted, please prioritize search	es in order of need.
Please provide a detailed statement of the search topic, and describe as specifical Include the elected species or structures, keywords, synonyms, acronyms, and randov & the invention. Define any terms that may have a special meaning. Given Please attach a copy of the cover sheet, pertinent claims, and abstract.	fly as possible the subject matter to be searched censury numbers, and combine with the concept or
Title of Invention: Benjamile This bishol	
Inventors (please provide full names):	
Earliest Priority Filing Date:	
For Sequence Searches Only Please include all pertinent information (parent, chi	
I seal opil I. (see dain)	X R', R' see sub
RZ O K	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
R3	
I sent apar of dan 10.	R4, R5, R1 que sub
I method of use of	
cpd Z	



STIC Search Report Biotech-Chem Library

STIC Database Tracking Number: 169801

TO: Rei-Tsang Shiao Location: 5a10 / 5c18

Monday, October 31, 2005

Art Unit: 1626

Phone: 571-272-0707

Serial Number: 10 / 748342

From: Jan Delaval

Location: Biotech-Chem Library

Remsen 1a51

Phone: 571-272-2504

jan.delaval@uspto.gov

Search Notes	





STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact the searcher or contact:

Mary Hale, Information Branch Supervisor 308-4258, CM1-1E01

Voluntary Results Feedback Form.
> I am an examiner in Workgroup: Example: 1610
> Relevant prior art found, search results used as follows:
☐ 102 rejection
☐ 103 rejection
Cited as being of interest.
Helped examiner better understand the invention.
Helped examiner better understand the state of the art in their technology.
Types of relevant prior art found:
Foreign Patent(s)
☐ Non-Patent Literature (journal articles, conference proceedings, new product announcements etc.)
> Relevant prior art not found:
Results verified the lack of relevant prior art (helped determine patentability).
Results were not useful in determining patentability or understanding the invention.
Comments:

Drop off or send completed forms to STIC/Biotech-Chem Library GM1 – Circ. Desk



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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 OCT 2005 HIGHEST RN 866393-44-4 DICTIONARY FILE UPDATES: 30 OCT 2005 HIGHEST RN 866393-44-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d sta que 19 L1 STR

VAR G3=15/22 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

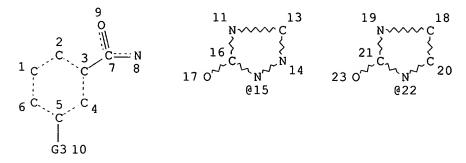
GRAPH ATTRIBUTES: RSPEC 1 13 18

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L3 124 SEA FILE=REGISTRY SSS FUL L1 L4

STR



VAR G3=15/22

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 2

CONNECT IS M1 RC AT 8

CONNECT IS M1 RC AT 11

CONNECT IS M1 RC AT 13

CONNECT IS M1 RC AT 18

CONNECT IS M1 RC AT 19

CONNECT IS M1 RC AT 20

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1 13 18

NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L6 35 SEA FILE=REGISTRY SUB=L3 CSS FUL L4

L7 17 SEA FILE=REGISTRY ABB=ON PLU=ON L6 AND 16.195.3/RID

PLU=ON L6 NOT L7 L8 18 SEA FILE=REGISTRY ABB=ON

L9 17 SEA FILE=REGISTRY ABB=ON PLU=ON L8 NOT C31H36CL3N5O4

=> d ide can 19 tot

L9 ANSWER 1 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-87-3 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxy-2-methylpropy1)-3-methyl-5oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

3D CONCORD FS

MF C22 H31 C1 N4 O4

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} Me & N & C1 \\ OH & N & C-NH-CH_2 \\ Me-C-CH_2 & O \\ Me & Me \end{array}$$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 2 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-86-2 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-[(2S)-2-hydroxy-3-methoxypropy1]-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H31 C1 N4 O5

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 3 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-85-1 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-[(2R)-2-hydroxy-3-methoxypropyl]-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]-

(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H31 C1 N4 O5

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 4 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-84-0 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 5-[4-(2-aminoethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-2-chloro-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H28 C1 N5 O3

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & O \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 5 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN RN 723242-83-9 REGISTRY

jan delaval - 31 october 2005

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxyethyl)-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H27 C1 N4 O4

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{C1} \\ \text{N} & \text{C} & \text{NH-CH}_2 \\ \text{HO-CH}_2 - \text{CH}_2 & \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 6 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-82-8 REGISTRY

ED Entered STN: 07 Aug 2004

CN 4H-1,2,4-Triazole-4-acetamide, 1-[4-chloro-3-[[(1-hydroxycycloheptyl)methyl]amino]carbonyl]phenyl]-1,5-dihydro-3-methyl-5-oxo-(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H26 C1 N5 O4

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 7 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN RN 723242-81-7 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-(2,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)-N- [(1-hydroxy-3,3-dimethylcyclohexyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H25 C1 N4 O3

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 8 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-80-6 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4-(cyanomethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H24 C1 N5 O3

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 9 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-79-3 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-methoxyethyl)-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX

NAME)

FS 3D CONCORD

MF C21 H29 C1 N4 O4

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & \\ & \\ MeO-CH_2-CH_2 \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 10 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-78-2 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4-(cyanomethyl)-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H22 C1 N5 O3

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 11 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-77-1 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxyethyl)-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C19 H25 C1 N4 O4

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ & & & \\ \text{HO-CH}_2-\text{CH}_2 & & \\ \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 12 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-76-0 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-(2,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C18 H23 C1 N4 O3

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{C1} \\ \text{N} & \text{C-NH-CH}_2 \\ \text{N} & \text{O} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 13 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-75-9 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl)-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS. 3D CONCORD

MF C17 H21 C1 N4 O3

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c}
 & C1 \\
 & C-NH-CH_2 \\
 & O \\
 & O
\end{array}$$

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 14 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 723242-74-8 REGISTRY

ED Entered STN: 07 Aug 2004

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-methoxyethyl)-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C20 H27 C1 N4 O4

SR CA

LC STN Files: CA, CAPLUS

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & \\ & O \end{array}$$
 MeO-CH₂-CH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:123633

L9 ANSWER 15 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 159545-52-5 REGISTRY

ED Entered STN: 14 Dec 1994

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(ethylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro-5-propyl[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C36 H44 F N5 O6 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:10037

L9 ANSWER 16 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 159545-50-3 REGISTRY

ED Entered STN: 14 Dec 1994

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C35 H42 F N5 O6 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1: 122:10037 REFERENCE

L9 ANSWER 17 OF 17 REGISTRY COPYRIGHT 2005 ACS on STN

RN 159545-48-9 REGISTRY

ED Entered STN: 14 Dec 1994

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
3D CONCORD

FS

MF C35 H43 N5 O6 S

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 122:10037

=> d his

(FILE 'HOME' ENTERED AT 12:06:49 ON 31 OCT 2005) SET COST OFF

FILE 'REGISTRY' ENTERED AT 12:06:54 ON 31 OCT 2005
L1 STR
L2 7 S L1
L3 124 S L1 FUL
SAV TEMP L3 SHIAO748/A
L4 STR L1
L5 2 S L4 CSS SAM SUB=L3

L6 35 S L4 CSS FUL SUB=L3 SAV L6 SHIAO748A/A TEMP

L7 17 S L6 AND 16.195.3/RID

L8 18 S L6 NOT L7

L9 17 S L8 NOT C31H36CL3N5O4 SAV L9 SHIAO748B/A

L10 18 S L6 NOT L9

FILE 'HCAOLD' ENTERED AT 12:14:27 ON 31 OCT 2005

L11 0 S L9 L12 0 S L10

FILE 'HCAPLUS' ENTERED AT 12:14:38 ON 31 OCT 2005 L13 2 S L9

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L14
              6 S L10
                E DOMBROSKI M/AU
L15
             40 S E3, E4, E9, E10
                E DUPLANTIER A/AU
L16
             29 S E3-E6
                E SUBRAMANYAM C/AU
L17
             73 S E3-E6, E8
L18
              1 S L13 AND L15-L17
L19
              0 S L14 AND L15-L17
L20
              1 S L13 AND PFIZER?/PA,CS
L21
              0 S L14 AND PFIZER?/PA,CS
L22
              2 S L13, L18, L20
L23
              6 S L14 NOT L22
     FILE 'USPATFULL, USPAT2' ENTERED AT 12:17:40 ON 31 OCT 2005
L24
              1 S L9
     FILE 'REGISTRY' ENTERED AT 12:18:09 ON 31 OCT 2005
=> fil uspatall
FILE 'USPATFULL' ENTERED AT 12:18:27 ON 31 OCT 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
FILE 'USPAT2' ENTERED AT 12:18:27 ON 31 OCT 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)
=> d 124 bib abs hitstr
    ANSWER 1 OF 1 USPATFULL on STN
L24
AN
       94:7707 USPATFULL
TI
       Substituted 1,2,4-triazoles bearing acidic functional groups as
       angiotensin II antagonists
ΙŃ
       Ashton, Wallace T., Clark, NJ, United States
       Chakravarty, Prasun K., Edison, NJ, United States
       Chang, Linda L., Wayne, NJ, United States
       Greenlee, William J., Teaneck, NJ, United States
       Kim, Dooseop, Scotch Plains, NJ, United States
       Mantlo, Nathan B., Westfield, NJ, United States
       Patchett, Arthur A., Westfield, NJ, United States
PA
       Merck & Co., Inc., Rahway, NJ, United States (U.S. corporation)
PΙ
      US 5281614
                               19940125
       US 1992-970360
ΑI
                               19921102 (7)
RLI
       Continuation-in-part of Ser. No. US 1992-875038, filed on 1 May 1992,
       now abandoned which is a continuation-in-part of Ser. No. US
       1991-698505, filed on 10 May 1991, now abandoned
DT
       Utility
FS
       Granted
EXNAM
      Primary Examiner: Tsang, Cecilia; Assistant Examiner: Gupta, Y. N.
LREP
       Camara, Valerie J., Daniel, Mark R., DiPrima, Joseph F.
CLMN
       Number of Claims: 11
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 5081
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB
       Novel substituted triazolinone, triazolinethione, and triazolinimine
       compounds of the formula I are useful as angiotensin II antagonists.
       ##STR1##
```

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 159545-48-9P 159545-50-3P 159545-52-5P

(preparation of, as angiotensin II antagonist)

RN 159545-48-9 USPATFULL CN Carbamic acid, [[4'-[[3]

Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl][1,1'-biphenyl]-2yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 159545-50-3 USPATFULL

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 159545-52-5 USPATFULL

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(ethylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro-5-propyl[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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FILE COVERS 1907 - 31 Oct 2005 VOL 143 ISS 19 FILE LAST UPDATED: 30 Oct 2005 (20051030/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d 113 all hitstr
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```
ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
L13
     2004:565226 HCAPLUS
AN
DN
     141:123633
ED
     Entered STN: 15 Jul 2004
ΤI
     Preparation of benzamide inhibitors of the P2x7 receptor
TN
     Duplantier, Allen J.; Subramanyam, Chakrapani; Dombroski, Mark A.
PΑ
     Pfizer Products Inc., USA
SO
     PCT Int. Appl., 79 pp.
     CODEN: PIXXD2
DΤ
     Patent
LA
     English
     ICM C07D249-12
IC
     ICS C07D233-70; A61K031-4196; A61P011-00; A61P037-00
CC
     28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1
FAN.CNT 1
     PATENT NO.
                               DATE
                                         APPLICATION NO.
                        KIND
                                                                 DATE
     -----
                                          -----
                        ____
                               _____
                                                                 _____
PΤ
    WO 2004058731
                        A1
                               20040715 WO 2003-IB6232
                                                                 20031230
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
            GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
            LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
            OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
            TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
            ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
            TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
                               20040715 CA 2003-2511189 20031230
20051005 EP 2003-780483 20031230
     CA 2511189
                        AA
     EP 1581507
                        Α1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRAI US 2002-437228P
                       P
                               20021231
    WO 2003-IB6232
                         W
                               20031230
CLASS
PATENT NO.
                CLASS PATENT FAMILY CLASSIFICATION CODES
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                ICS
                       C07D233-70; A61K031-4196; A61P011-00; A61P037-00
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                       C07D233/70; C07D249/12
CA 2511189
                ECLA
                       C07D233/70; C07D249/12
EP 1581507
                ECLA
                       C07D233/70; C07D249/12
os
    MARPAT 141:123633
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AB
     Title benzamide derivs. I (R1 = alkyl, optionally substituted by
     cycloalkyl, aryl, heteroaryl; R2 = H, halo, cyano, optionally substituted
     alkyl; R3 = suitably substituted nitrogen-linked heterocyclyl) and
     pharmaceutically acceptable salts, useful as P2X7 receptor antagonists,
     are prepared Thus, 2-chloro-N-(1-hydroxycycloheptylmethyl)-5-[4-(2-
     methoxyethyl)-5-oxo-4,5-dihydro[1,2,4]triazol-1-yl]benzamide was prepared in
     a multi-step synthesis from 5-amino-2-chlorobenzoic acid. The compds. of
     the invention are useful in the treatment of IL-1 mediated disorders,
     including, without limitation, inflammatory diseases such as
     osteoarthritis and rheumatoid arthritis; allergies, asthma, COPD, cancer,
     reperfusion or ischemia in stroke or heart attack, autoimmune diseases and
     other disorders.
ST
     benzamide triazolyl prepn purinergic receptor antagonist
ΙT
     Purinoceptor antagonists
        (P2x7; preparation of benzamide inhibitors of the P2x7 receptor)
IT
     Purinoceptors
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (P2x7; preparation of benzamide inhibitors of the P2x7 receptor)
IΤ
     Interleukin 1
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of benzamide derivs. for treatment of IL-1 mediated disease)
TΤ
     89-54-3, 5-Amino-2-chlorobenzoic acid
                                             298-12-4, Oxoacetic acid
     2815-39-6
                 6482-24-2, 2-Bromoethyl methyl ether
                                                        26386-88-9,
     Diphenylphosphoryl azide
                                64491-70-9, (R)-Glycidyl methyl ether
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of benzamide inhibitors of the P2x7 receptor)
IΤ
     42122-75-8P, 5-Amino-2-chlorobenzoic acid methyl ester
                                                              723242-88-4P
     723242-89-5P
                    723242-90-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of benzamide inhibitors of the P2x7 receptor)
IT
     723242-74-8P 723242-75-9P 723242-76-0P
     723242-77-1P 723242-78-2P 723242-79-3P
     723242-80-6P 723242-81-7P 723242-82-8P
     723242-83-9P 723242-84-0P 723242-85-1P
     723242-86-2P 723242-87-3P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of benzamide inhibitors of the P2x7 receptor)
TΤ
     723242-74-8P 723242-75-9P 723242-76-0P
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     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of benzamide inhibitors of the P2x7 receptor)
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     723242-74-8 HCAPLUS
CN
     Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-methoxyethyl)-5-oxo-1H-1,2,4-
     triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)
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$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

RN 723242-75-9 HCAPLUS

CN Benzamide, 2-chloro-5-(2,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl)-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & & \\$$

RN 723242-76-0 HCAPLUS

CN Benzamide, 2-chloro-5-(2,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{C1} \\ \text{N} & \text{C-NH-CH}_2 \\ \text{N} & \text{O} \end{array}$$

RN 723242-77-1 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxyethyl)-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 723242-78-2 HCAPLUS

CN Benzamide, 2-chloro-5-[4-(cyanomethyl)-4,5-dihydro-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

RN 723242-79-3 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-methoxyethyl)-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & O \end{array}$$

RN 723242-80-6 HCAPLUS

CN Benzamide, 2-chloro-5-[4-(cyanomethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

Me N C1
$$C-NH-CH_2$$
 O $NC-CH_2$ O

RN 723242-81-7 HCAPLUS

CN Benzamide, 2-chloro-5-(2,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl)-N- [(1-hydroxy-3,3-dimethylcyclohexyl)methyl]- (9CI) (CA INDEX NAME)

RN 723242-82-8 HCAPLUS

CN 4H-1,2,4-Triazole-4-acetamide, 1-[4-chloro-3-[[[(1-hydroxycycloheptyl)methyl]amino]carbonyl]phenyl]-1,5-dihydro-3-methyl-5-oxo-(9CI) (CA INDEX NAME)

RN 723242-83-9 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxyethyl)-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

RN 723242-84-0 HCAPLUS

CN Benzamide, 5-[4-(2-aminoethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-2-chloro-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & O \end{array}$$

RN 723242-85-1 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-[(2R)-2-hydroxy-3-methoxypropyl]-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 723242-86-2 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-[(2S)-2-hydroxy-3-methoxypropyl]-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 723242-87-3 HCAPLUS

CN Benzamide, 2-chloro-5-[4,5-dihydro-4-(2-hydroxy-2-methylpropyl)-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl]-N-[(1-hydroxycycloheptyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 \\ & C-NH-CH_2 \\ & OH \\ & N \\ & OH \\ &$$

L13 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

TI Preparation of substituted 1,2,4-triazoles bearing acidic functional groups as angiotensin II antagonists

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IN
     Ashton, Wallace T.; Chakravarty, Prasun K.; Chang, Linda L.; Greenlee,
     William J.; Kim, Dooseop; Mantlo, Nathan B.; Patchett, Arthur A.
     1995:234501 HCAPLUS
ΑN
DN
     122:10037
ED
     Entered STN: 10 Dec 1994
TΤ
     Preparation of substituted 1,2,4-triazoles bearing acidic functional
     groups as angiotensin II antagonists
     Ashton, Wallace T.; Chakravarty, Prasun K.; Chang, Linda L.; Greenlee,
TN
     William J.; Kim, Dooseop; Mantlo, Nathan B.; Patchett, Arthur A.
PA
     Merck and Co., Inc., USA
SO
     U.S., 75 pp. Cont.-in-part of U.S. Ser. No. 875,038, abandoned.
     CODEN: USXXAM
DT
     Patent
    English
LA
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     ICM A61K031-41
     ICS A61K031-505; A61K031-535; C07D249-10; C07D249-12; C07D249-14
INCL 514359000
     28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1, 63
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                       514/343.000; 514/361.000; 514/362.000; 514/364.000;
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US 5436259
                       514/384.000; 514/359.000; 548/262.800; 548/263.200;
                NCL
                       548/264.600
                       C07D249/12; C07D413/10+271+249; C07D417/10+285+249;
                ECLA
                       C07D417/10+285B+249; C07D419/10+291+249
os
    MARPAT 122:10037
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$$R^{6E}$$
 R^{3a}
 R^{3a}
 R^{2a}
 R^{2a}
 R^{2b}
 R^{2b}
 R^{2b}

AB Title compds. I [R1 = R22SO2NHSO2, R22O2CNHSO2, NCNHSO2, (R24)2P(O)NHSO2,R24P(O)NHCO, substituted heterocyclyl wherein R22 = (substituted) Ph, -C1-6 alkyl, -C2-6 alkenyl, -C2-6 alkynyl, heteroaryl, (substituted) C3-7 cycloalkyl, etc., R24 = aryl , (substituted) C1-6 alkyl, etc.; R2a, R2b = H, halo, (substituted) amino, O2N, F3C, (substituted) C1-6 alkyl, heterocyclyl, etc., R2aR2b = Ph; R3a = H, halo, C1-6 alkyl, C1-6 alkoxy, etc.; R3b = H, halo, C1-6 alkyl, C1-5 alkylcarbonyloxy, C3-5 cycloalkyl, C1-6 alkoxy, etc, R3aR3b = Ph, biphenyl, (substituted) naphthyl; A = O, S, R21N wherein R21 = H, (substituted) Ph, -C1-6 alkyl, etc.; B = (substituted) C1-10 alkyl, halo, H, (substituted) aryl, etc.; E = bond, (substituted) amino, alkylsulfonyl, CHOH, alkoxy, CO; R6 = (substituted) Ph, -C1-6 alkyl, -heteroaryl, -C3-7 cycloalkyl, etc.; X = bond, CO, O, S, etc.; u = 1,2] or a salt thereof, showing activity as angiotensin II antagonists, are prepared N-[[2'-carboxybiphenyl-4-yl]methyl]phthalimide (preparation given) was converted in 4 steps to 4-[[2'-(tertbutoxycarbonyl)biphenyl-4-yl]-5-n-butyl]-2,4-dihydro-3H-1,2,4-triazole-3thione which was treated with F3CCO2H to give I (R1 = HO2C, A = S, B = R2a= R2b = R3a = R3b = H, R6E = Bu, X = bond, u = 1). ST triazole substituted prepn angiotensin antagonist; butylcarboxybiphenylyl

triazolethione prepn angiotensin antagonist IT Nervous system agents

(substituted triazoles)

IT Antihypertensives

(substituted triazoles as, angiotensin II receptor antagonists in relation to)

IT Glaucoma (disease)

(treatment of. substituted triazoles for)

IT Receptors

RL: BSU (Biological study, unclassified); BIOL (Biological study) (angiotensin II, antagonists, substituted triazoles)

IT 937-12-2P, p-Tolyltrimethyltin 999-09-7P, Ethyl valerimidate 40872-87-5P 83483-30-1P, Ethyl N-carbethoxyvalerimidate 89981-25-9P 133690-72-9P 133690-73-0P 133690-74-1P 133690-75-2P 133690-76-3P 133690-79-6P 133690-78-5P 133690-92-3P 133690-91-2P 138733-50-3P 138733-51-4P 138733-52-5P 145004-90-6P 145004-91-7P 145004-92-8P 146948-92-7P 146948-93-8P 146948-94-9P 146948-95-0P 146948-96-1P 146949-00-0P 146948-97-2P 146948-98-3P 146948-99-4P 146949-01-1P 146949-02-2P 146949-03-3P 146949-04-4P 146949-05-5P 147776-48-5P

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     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and reaction of, in preparation of angiotensin II antagonists)
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                                                                    159546-68-6P
     159546-69-7P
                    159546-70-0P
                                    159546-71-1P
                                                    159546-72-2P
                                                                    159546-73-3P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
```

```
(preparation of, as angiotensin II antagonist)
TT
     159546-74-4P
                   159546-75-5P
                                   159546-76-6P
                                                  159546-77-7P
                                                                 159546-78-8P
     159546-79-9P
                    159546-80-2P
                                   159546-81-3P
                                                  159546-82-4P
                                                                 159546-83-5P
     159546-84-6P
                    159546-85-7P
                                   159546-86-8P
                                                  159546-87-9P
                                                                 159546-88-0P
     159546-89-1P
                    159546-90-4P
                                   159546-91-5P
                                                  159546-92-6P
                                                                 159546-93-7P
     159546-94-8P
                   159546-95-9P
                                   159546-96-0P
                                                  159546-97-1P
                                                                 159546-98-2P
     159546-99-3P
                    159547-00-9P
                                   159547-01-0P
                                                  159547-02-1P
                                                                 159547-03-2P
     159547-04-3P
                    159547-05-4P
                                   159547-06-5P
                                                  159547-07-6P
                                                                 159547-08-7P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of, as angiotensin II antagonist)
IΤ
     75-64-9, tert-Butylamine, reactions
                                          100-63-0, Phenylhydrazine
     104-81-4, 4-Methylbenzyl bromide
                                       358-23-6, Trifluoromethanesulfonic
     anhydride
                365-34-4, 2-(Trifluoromethyl)phenylhydrazine
                                                                541-41-3, Ethyl
     chloroformate
                     627-03-2, Ethoxyacetic acid 627-04-3, Ethylthioacetic
           638-29-9, Valeryl chloride
                                        1066-45-1, Trimethyltin chloride
     1074-82-4, Potassium phthalimide
                                       1514-87-0, Methyl chlorodifluoroacetate
     2905-25-1
                 4114-31-2, Ethyl carbazate
                                              4294-57-9, p-Tolylmagnesium
              5419-55-6, Triisopropyl borate 10147-37-2, Isopropylsulfonyl
    bromide
               10449-07-7, o-Chlorophenylhydrazine
                                                      13360-57-1,
     Dimethylsulfamoyl chloride 13820-09-2, Trimethyl orthovalerate
     18542-63-7, Ethyl valerimidate hydrochloride
                                                    24424-99-5, Di-tert-butyl
     dicarbonate
                  39684-28-1, O-tert-Butylhydroxylamine-hydrochloride
     51436-99-8, 4-Bromo-2-fluorotoluene
                                           76283-09-5, 4-Bromo-2-fluorobenzyl
               96701-59-6, (2-Chloro-5-nitrophenyl) hydrazine
                                                              100367-78-0
     114772-40-6, 4-(Bromomethyl)-2'-(tert-butoxycarbonyl)biphenyl
     114772-54-2, 4-(Bromomethyl)-2'-cyanobiphenyl
                                                    133690-87-6
                                                                   146949-07-7,
     4-Propylbenzenesulfonyl chloride
                                        146949-08-8, 4-Nitro-2-
                                       150691-04-6
     (trifluoromethyl)phenylhydrazine
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, in preparation of angiotensin II antagonists)
TΤ
     11128-99-7, Angiotensin II
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (receptors for, antagonists, substituted triazoles)
IT
     159545-48-9P 159545-50-3P 159545-52-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of, as angiotensin II antagonist)
     159545-48-9 HCAPLUS
RN
CN
     Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5-
     dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl][1,1'-biphenyl]-2-yl]sulfonyl]-
     , 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
```

RN 159545-50-3 HCAPLUS

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(butylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 159545-52-5 HCAPLUS

CN Carbamic acid, [[4'-[[3-butyl-1-[3-[(ethylamino)carbonyl]phenyl]-1,5-dihydro-5-oxo-4H-1,2,4-triazol-4-yl]methyl]-3'-fluoro-5-propyl[1,1'-biphenyl]-2-yl]sulfonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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STRUCTURE FILE UPDATES: 30 OCT 2005 HIGHEST RN 866393-44-4 DICTIONARY FILE UPDATES: 30 OCT 2005 HIGHEST RN 866393-44-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and

jan delaval - 31 october 2005

predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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L10 ANSWER 1 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 856901-99-0 REGISTRY

ED Entered STN: 25 Jul 2005

CN Benzamide, N-(3-cyclobutyl-2,3,4,5-tetrahydro-1H-3-benzazepin-7-yl)-3-(2-oxo-1-imidazolidinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H28 N4 O2

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 143:97280

L10 ANSWER 2 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 616244-55-4 REGISTRY

ED Entered STN: 13 Nov 2003

CN Benzamide, N-[2,3-bis(4-chlorophenyl)-1-methylpropyl]-3-(2-oxo-1-imidazolidinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C26 H25 C12 N3 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:337785

L10 ANSWER 3 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 616243-51-7 REGISTRY

ED Entered STN: 13 Nov 2003

CN Benzamide, N-[(1R, 2R)-2, 3-bis(4-chlorophenyl)-1-methylpropyl]-3-(2-oxo-1-methylpropyl)-3-

imidazolidinyl)-, rel- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H25 C12 N3 O2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:337785

L10 ANSWER 4 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 340188-12-7 REGISTRY

ED Entered STN: 08 Jun 2001

CN Glycine, N-[3-[(4S)-4-(3-aminopropyl)-2,5-dioxo-1-imidazolidinyl]benzoyl]- L- α -aspartyl-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H27 N5 O8

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:360991

L10 ANSWER 5 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 340188-11-6 REGISTRY

ED Entered STN: 08 Jun 2001

CN Glycine, N-[3-[(4S)-4-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl-2-phenyl-, bis(1,1-dimethylethyl) ester, (2S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C38 H51 N5 O10

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:360991

L10 ANSWER 6 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-14-2 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C32 H39 N5 O10

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 7 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-12-0 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-(acetylamino)propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C29 H33 N5 O9

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 8 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-11-9 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[[[imino[(methoxycarbonyl)amino]methyl]amino]methyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C32 H39 N7 O10

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 9 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-10-8 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[[(aminoiminomethyl)amino]methyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C30 H37 N7 O8

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 10 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-09-5 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-(acetylamino)propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C33 H41 N5 O9

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

- 1 REFERENCES IN FILE CA (1907 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

jan delaval - 31 october 2005

REFERENCE 1: 121:180236

L10 ANSWER 11 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-08-4 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-(acetylamino)propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C27 H29 N5 O9

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 12 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157702-06-2 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-[[[1-(acetyloxy)ethoxy]carbonyl]amino]propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C32 H37 N5 O12

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 13 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157701-98-9 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-(3-aminopropyl)-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C27 H31 N5 O8

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 14 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 157701-97-8 REGISTRY

ED Entered STN: 16 Sep 1994

CN Glycine, N-[N-[3-[4-[3-[(methoxycarbonyl)amino]propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-L-2-phenyl-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C29 H33 N5 O10

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 121:180236

L10 ANSWER 15 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 150376-47-9 REGISTRY

ED Entered STN: 01 Oct 1993

CN L-Valine, N-[N-[3-[4-[3-[[imino(nitroamino)methyl]amino]propyl]-2,5-dioxo-l-imidazolidinyl]benzoyl]-L- α -aspartyl]-, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C23 H30 N8 O10

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

jan delaval - 31 october 2005

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 119:181238

L10 ANSWER 16 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 150376-46-8 REGISTRY

ED Entered STN: 01 Oct 1993

CN L-Valine, N-[N-[3-[4-[3-[[imino(nitroamino)methyl]amino]propyl]-2,5-dioxo-l-imidazolidinyl]benzoyl]-L- α -aspartyl]-, bis(1,1-dimethylethyl) ester, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C31 H46 N8 O10

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 119:181238

L10 ANSWER 17 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 150376-11-7 REGISTRY

ED Entered STN: 01 Oct 1993

CN L-Valine, N-[N-[3-[4-[3-[(aminoiminomethyl)amino]propyl]-2,5-dioxo-1-imidazolidinyl]benzoyl]-L- α -aspartyl]-, (S)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE

MF C23 H31 N7 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 119:181238

L10 ANSWER 18 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN

RN 75955-94-1 REGISTRY

ED Entered STN: 16 Nov 1984

CN Benzamide, N-[4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]-3-(3-dodecyl-2,5-dioxo-1-imidazolidinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C31 H36 C13 N5 O4

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 94:22896

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FILE 'REGISTRY' ENTERED AT 12:06:54 ON 31 OCT 2005

L1 STR

L2 7 S L1

L3 124 S L1 FUL

SAV TEMP L3 SHIAO748/A

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L4
                STR L1
L5
              2 S L4 CSS SAM SUB=L3
L6
             35 S L4 CSS FUL SUB=L3
                SAV L6 SHIAO748A/A TEMP
L7
             17 S L6 AND 16.195.3/RID
L8
             18 S L6 NOT L7
L9
             17 S L8 NOT C31H36CL3N5O4
                SAV L9 SHIAO748B/A
L10
             18 S L6 NOT L9
     FILE 'HCAOLD' ENTERED AT 12:14:27 ON 31 OCT 2005
L11
              0 S L9
L12
              0 S L10
     FILE 'HCAPLUS' ENTERED AT 12:14:38 ON 31 OCT 2005
              2 S L9
L13
L14
              6 S L10
                E DOMBROSKI M/AU
L15
             40 S E3, E4, E9, E10
                E DUPLANTIER A/AU
L16
             29 S E3-E6
                E SUBRAMANYAM C/AU
L17
             73 S E3-E6, E8
L18
             1 S L13 AND L15-L17
L19
             0 S L14 AND L15-L17
L20
              1 S L13 AND PFIZER?/PA,CS
L21
              O S L14 AND PFIZER?/PA,CS
L22
              2 S L13, L18, L20
L23
              6 S L14 NOT L22
     FILE 'USPATFULL, USPAT2' ENTERED AT 12:17:40 ON 31 OCT 2005
L24
              1 S L9
     FILE 'REGISTRY' ENTERED AT 12:18:09 ON 31 OCT 2005
     FILE 'USPATFULL, USPAT2' ENTERED AT 12:18:27 ON 31 OCT 2005
     FILE 'HCAPLUS' ENTERED AT 12:18:43 ON 31 OCT 2005
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FILE 'REGISTRY' ENTERED AT 12:21:40 ON 31 OCT 2005

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